Recommendations for Presentation of Kinetic and Photochemical Data

Overview

The evaluation of chemical kinetic and photochemical data to provide an analysis of the most reliable parameters and their associated error estimates is a challenging task. It usually requires a meta-analysis of results from several experiments, where individual rate or cross section parameter determinations from various studies are plotted as a function of one or more experimental variables (temperature, pressure, photolysis wavelength, surface composition, etc.) Such plots are difficult or impossible to construct and interpret if the data in the original publications are presented in either an incomplete or ambiguous fashion. The recommendations presented below are addressed to those who prepare manuscripts presenting experimental chemical kinetic or photochemical data for publication and to those who review and edit such manuscripts before their publication. You cooperation in ensuring these manuscripts present their results in a clear and complete manner will make subsequent data evaluation tasks significantly easier and more accurate. Without your cooperation there is no way that all relevant data can be properly included in the recommendations presented to the user community.

Data Presentation

It is extremely important that all individual target quantities (rate constants, cross sections, quantum yields, etc.) be published in a tabular form that includes specification of critical experimental parameters (e.g. temperature, pressure, wavelength, surface composition for heterogeneous processes, pH or other concentration/activity parameters for liquid phase reactions). Data plots as a function of one or more critical experimental parameters are usually both enlightening and edifying. However, data plots alone will not suffice. Picking points from data plots is both difficult and imprecise, making it extremely hard to accurately compare the data with those from other studies. If space limitations or inappropriate editorial pressure makes it difficult to present complete data tables in the published text, then they should be included as supplementary material on the journal's web site. However, since the future accessibility of supplementary material is less certain than the data presented in the primary publication, as much tabular data as possible should be included in the main text.

Data Certification

When an individual researcher or research group publishes multiple studies on the same process, it is critical that they clearly state the differences between the studies, and which prior data are superseded by subsequent data. Publishing a second set of data covering the same variable space without clearly stating whether prior data are either included in or invalidated by a second (or nth) study is unacceptable. In such cases there is no way a data reviewer/evaluator can clearly determine which data to include without a clear declaration from the originating authors of multiple publications certifying which data represent their best effort to the date of publication.

Error Analysis

Data presented without error estimates are useless. It is incumbent on all researchers to prepare and present a thorough analysis of the errors associated with their measurements. This analysis should include both statistical and estimated systematic errors. Computed statistical errors should always indicate what level of uncertainty (1 σ, 2 σ, etc.) they represent. Honest estimates of quantifiable systematic errors should be articulated, presented, and then appropriately combined with computed statistical errors to indicate total measurement uncertainties. All data presented in published text and associated data tables should include numerical uncertainty estimates that are consistent throughout the publication. All plotted data points should include appropriate and consistent error bars. A full and clear explanation of the uncertainty ranges and error bars presented and/or plotted should be presented in every publication.

Summary

The determination and publication of accurate kinetic and photochemical parameters are usually expensive and time-consuming tasks. When these tasks are well done the data obtained and presented can have lasting value that is greatly enhanced when it can be accurately compared and combined with data from similar studies. If authors take care to fully publish their data, certify how the results from multiple studies relate, and present a thorough and consistent error analysis, the full value of their data can be assessed and transmitted to the user community.